Supersymmetry approach to nuclear-spin-polarization-induced quantum dot structure calculations

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In nuclear-spin-polarization-induced quantum dots the electrons are confined through local nuclear spin polarization. The model electron confinement potential is time-dependent due to the nuclear spin diffusion and relaxation processes. It can be well-approximated by a Gaussian curve which is not an exactly solvable potential. We demonstrate that it can also be approximated by multisoliton potentials for the zero value of the angular momentum and by their singular analogues for other values of momentum without any loss of calculational accuracy. We obtain these potentials by supersymmetric (or equivalently Darboux) transformations from the zero potential. The main advantage of such potentials is that they are exactly solvable. Time-dependence of the nuclear-spin-polarization-induced quantum dot energy levels is found.

I. INTRODUCTION

In recent times theoretical and experimental investigations of quantum dots is attracting a considerable attention [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. In particular, it has been suggested that a novel class of quantum dots [10, 11], so-called nuclear-spin-polarization-induced (NSPI) quantum dots (QD), as well as other NSPI low-dimensional electron structures [13, 14, 15], could be created through locally polarized nuclear spins. The main idea of creating NSPI structures consists of the following. Electron and nuclear spins interact via the contact hyperfine interaction that can be described by an effective hyperfine field $\mathbf{B}_{hf}$, which acts at spins of electrons and contributes to the electronic Hamiltonian through a Zeeman-type potential $g^*\mu_B\sigma\mathbf{B}_{hf}(\mathbf{r},t)/2$ [16]. (Here g^* is the effective electron g-factor, μ_B is the Bohr magneton and σ is the Pauli matrix-vector). The Zeeman splitting results in the potential that is attractive for the electrons with one spin projection and repulsive for others. In this model the energy is shifted by a constant of the order of the Fermi energy by means of a gate. Then the potential, created by the inhomogeneous nuclear spin polarization

$$U_{conf}(\mathbf{r},t) = -\frac{|g^*|}{2}\mu_B B_{hf}(\mathbf{r},t) \qquad (1)$$

is confining. It is assumed that $B_{hf}(\mathbf{r},t) > 0$.

The idea to create NSPI QDs has been proposed for the first time by Fleurov et al [10]. They used a perturbation theory to find the modification of the energy spectrum of a traditional quantum dot due to the polarized nuclear spins. Formalism describing NSPI structures was thereafter developed and used in investigations of NSPI

quantum wires [13]. It was established that properties of NSPI structures are time-dependent because of nuclear spin diffusion and relaxation processes. Subsequently, this formalism has been used to investigate NSPI quantum dots [11], NSPI quantum rings [14], and NSPI periodic structures [15]. Moreover, related low-dimensional electron structures created through modulation of spin-orbit interaction coupling constant have also been considered [12].

It was assumed in [11] that a NSPI QD is created in the region of the intersection of the two-dimensional electron gas with cylindrically polarized nuclear spins. The electron energy levels at any particular time were found as a solution of the 2D radial Shrödinger equation with a Gaussian confining potential. The 2D radial Shrödinger equation (as well as 3D one) with a Gaussian potential does not give analytic solutions. Different methods were used to solve this problem [17, 18, 19, 20, 21]. A parabolic approximation of the Gaussian potential has been used in Ref. [11]. However, such an approximation is acceptable only for the ground state [11, 17].

In this paper we extend the study of NSPI systems by considering NSPI QD created through spherically polarized nuclear spins. Time dependence of the electron confining potential of Gaussian type is found as a solution of the diffusion equation with a relaxation term and the problem is thus reduced to solving the 3D radial Shrödinger equation where the time is involved as a parameter. For the zero value of the angular momentum we approximate the Gaussian potential, which is not exactly solvable, by a multisoliton potential, which is exactly solvable. The multisoliton potential is obtained by the technique of supersymmetric quantum mechanics (or

equivalently by the method of Darboux transformations). For other angular momenta the method gives their singular analogues. It should be mentioned that the applicability of our approach is not restricted only to NSPI QDs. It could be used for describing traditional quantum dots [17] also.

The paper is organized as follows. We introduce the basic equations describing NSPI QD in Sec. II. In Sec. III we present the method of calculations. Time dependence of the electron states in NSPI QD is studied in Sec. IV. The conclusions are drawn in Sec. V.

II. BASIC EQUATIONS

Let us consider a semiconductor structure with locally polarized nuclear spins. There are two main mechanisms leading to the time dependence of the hyperfine field describing the nuclear spin polarization: nuclear spin relaxation and nuclear spin diffusion. Then the evolution of the hyperfine field is governed by the diffusion equation

$$\frac{\partial B_{hf}}{\partial t} = D\Delta B_{hf} - \frac{1}{T_1} B_{hf} \qquad (2)$$

accounting also for the relaxation processes [13]. Here D is the spin-diffusion coefficient, Δ is the usual three-dimensional Laplacian, and T_1 is nuclear spin relaxation time [16, 22]. In the simplest case, we can assume a Gaussian form $B_{hf}(r, 0) = B_0 \exp\left(-\frac{r^2}{2d^2}\right)$ for the initial condition. The parameters d and B_0 define the half-width and the amplitude of the initial distribution of the hyperfine field respectively. Then the solution of Eq. (2) is:

$$B_{hf}(r, t) = B_0 e^{-\frac{t}{T_1}} \left(1 + \frac{t}{t_0}\right)^{-\frac{3}{2}} e^{-\frac{r^2}{2d^2\left(1 + \frac{t}{t_0}\right)}}, \qquad (3)$$

where $t_0 = \frac{d^2}{2D}$. The maximum nuclear field in GaAs can be as high as $B_{hf} = 5.3T$ in the limit that all nuclear spins are fully polarized [23]. This high level of nuclear spin polarization has been achieved experimentally. For example, the optical pumping of nuclear spins in 2DEG has demonstrated the nuclear spin polarization of the order of 90% [24]. A similar high polarization has been created by quantum Hall edge states (85%) [25]. These techniques are developed to allow local polarization and controllability of nuclear spins [26].

Our approach is based on the following electronic Hamiltonian:

$$H = -\frac{\hbar^2}{2m^*}\Delta - \frac{|g^*|}{2}\mu_B B_{hf}(\mathbf{r}, t), \qquad (4)$$

where m^* is the electron effective mass. The time scale introduced by the nuclear spins is several orders of magnitude larger than the time scale of typical electron equilibration processes. In such a case the electrons feel a quasi-constant average nuclear field. This simplifies calculation by avoiding the complications which would appear when solving the Schrödinger equation with the time dependence due to polarized nuclei. We take into account only the electrons with the spins along the z axis, for which the effective potential is attractive.

The electron energy levels in NSPI QD are determined by the radial Schrödinger equation that in appropriate units takes the form

$$\left[-\frac{d^2}{dx^2} + V^{(l)}(x, t) - E\right]\psi_{n,l}(x, t) = 0, \qquad (5)$$

where $\psi_{n,l}(x, t)$ is related with the radial part of the wave function $R_{n,l}(x, t)$ as follows: $\psi_{n,l}(x, t) = xR_{n,l}(x, t)$,

$$V^{(l)}(x, t) = \frac{l(l+1)}{x^2} - \gamma\frac{B_{hf}(x, t)}{B_{hf}(0, 0)}, \qquad (6)$$

$x = r/d$, $\gamma = |g^*|\mu_B B_{hf}(0, 0)/(2E_0)$, $E = \varepsilon/E_0$ is the energy in dimensionless units, ε is the energy, $E_0 = \hbar^2/(2m^*d^2)$, and $l = 0, 1, \ldots$. In the next Section we describe the method we are using to approximate the potential (6) with the effective hyperfine field B given by Eq. (3).

III. METHOD OF CALCULATION

The Darboux transformation method also known as the method of supersymmetric quantum mechanics is an effective tool for solving different problems of theoretical and mathematical physics (for reviews see [27]). Here we are using its property to approximate an interaction between composite particles by a local potential with an experimental accuracy, which previously proved to be very efficient in describing iso-phase (also known as phase equivalent) potentials in nuclear physics [28, 29]. Below we outline shortly the main features of the method we need.

Suppose one knows all solutions of the Schrödinger equation with a given reference potential V_0

$$h_0\psi = E\psi, \quad h_0 = -\frac{d^2}{dx^2} + V_0(x). \qquad (7)$$

Then, using a simple algorithm, one can construct a huge multiparameter family of exactly solvable potentials. The solutions φ of the Schrödinger equation with these potentials are obtained by acting on solutions of h_0 with a differential operator, $\varphi = L\psi$. In the simplest case this is a first order operator

$$L = -d/dx + w(x), \qquad (8)$$

where the real function $w(x)$ (known in supersymmetric quantum mechanics as *superpotential*) is defined as the logarithmic derivative of a solution u of (7). So, one has

$$w = u'(x)/u(x), \quad h_0 u = \alpha u, \qquad (9)$$

with $\alpha \leq E_0$, where E_0 is the ground state energy of h_0 if it has a discrete spectrum or the lower bound of the continuous spectrum. The function u is called *transformation* or *factorization function* and α its *factorization constant* or *factorization energy*. The potential V_1 of the Hamiltonian $h_1 = -d^2/dx^2 + V_1$, $h_1\varphi = E\varphi$, is defined in terms of the superpotential w as

$$V_1(x) = V_0(x) - 2w'(x).\tag{10}$$

Eq. (8) defines a first order Darboux transformation. In the following we shall deal with chains of N successive transformations of this type.

Here we will use very special chains introduced in [29]. They are generated by the following system of transformation functions

$$v_1(x),\ldots,v_l(x),u_{l+1}(x),v_{l+1}(x),\ldots,u_n(x),v_n(x)\tag{11}$$
$$h_0 u_j(x) = -a_j^2 u_j(x),\quad h_0 v_j(x) = -b_j^2 v_j(x),\tag{12}$$

where v_j are regular ($v_j(0) = 0$) and u_j irregular ($u_j(0) \neq 0$) at the origin. They have arbitrary eigenvalues $-a_j{}^2$ and $-b_j{}^2$ respectively, but always below E_0. If we are interested in the final action of the chain only, the solution $\psi_N(x,k)$ of the transformed equation with the Hamiltonian

$$h_N = -d^2/dx^2 + V_N\tag{13}$$

corresponding to the energy $E = k^2$ is given by [30]

$$\psi_N(x,k) = W(u_1,\ldots,u_n,\psi_0(x,k))\,W^{-1}(u_1,\ldots,u_N)\tag{14}$$

where W are Wronskians expressed in terms of u_j, denoting symbolically any function of (11) and of $\psi_0(x,k)$ which is a solution of the original Schrödinger equation corresponding to the same energy E, $N = 2n - l$. In the Hamiltonian (13) the transformed potential is

$$V_N = V_0 - 2\frac{d^2}{dx^2}\ln W(u_1,\ldots,u_N).\tag{15}$$

For $N = 1$ one has $W(u_1) \equiv u_1$ and one recovers (10) with $u = u_1$. If V_0 is finite at the origin, V_N behaves as $l(l+1)x^{-2}$ when $x \to 0$. Therefore the parameter l can be associated with the value of the angular momentum in (6). The formulas (14) and (15) result from the replacement of a chain of N first order transformations by a single Nth order transformation, which happens to be more efficient in practical calculations.

In Ref. [29] we obtained that the transformed Jost function F_N is related to the initial Jost function F_0 by

$$F_N(k) = F_0(k) \prod_{j=1}^{l}\frac{k}{k+ib_j}\prod_{j=l+1}^{n}\frac{k-ia_j}{k+ib_j}.\tag{16}$$

For $l = 0$ the first product is unity. Since a Jost function is analytic in the upper half of the complex k-plane (see e. g. [31]) all b's must be positive whereas the a's can
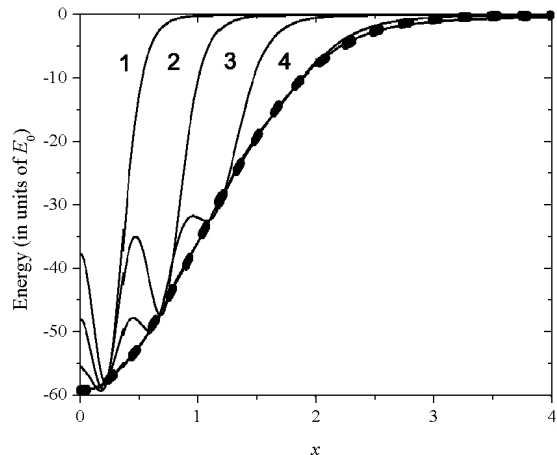

FIG. 1: Comparison between different multisoliton potentials. 1: two soliton, 2: four soliton, 3: six soliton, 4: eight and ten soliton, bold dashed line represent the Gaussian potential.

have any sign, so that every positive a_j corresponds to a discrete level $E = -a_j^2$ of h_N.

In our case we choose $V_0 = 0$ so that only exponentials are involved in the final Hamiltonian. Moreover, since the potential (6) is symmetric with respect to inversion $x \to -x$ we take $u_j(x) = \cosh(a_j x)$ and $v_j = \sinh(b_j x)$. In this case for $l = 0$ we get symmetric multisoliton potentials (see e.g. the first of Refs. [27]). Moreover, the Wronskian from (15) can be expressed as a sum of hyperbolic cosines [32]. For $l > 0$ we get singular at the origin analogues of multisoliton potentials. To compare them with the second term of the right hand side of (6) we have to subtract the centrifugal part and consider $V_{eff} = V_N - l(l+1)x^{-2}$. The potential V_{eff} depends on $N = 2n - l$ parameters a_j and b_j which we fit to the Gaussian curve of the second term of the right hand side of (6) for all values of t. This gives us the time dependence of the parameters a_j and b_j and hence the energy levels $E_j = -a_j^2$. To get an idea how many functions of type (11) could be involved in a particular case, we plotted the potentials (15) for $N = 2, 4, \ldots, 10$, $l = 0$, $B_0 = 1, t_0/T_1 = 1, \tau = 0$ in Fig. 1. It is clearly seen from this figure the solitonic structure of the curves for $N < 8$ (curves 1, 2 and 3). The result for $N = 8$ (curve 4) is not distinguishable of that for $N = 10$ and practically coincides with the given Gaussian potential curve. Moreover, for $N = 10$ the highest energy level is equal to zero with a high precision. This indicates that this potential has only four discrete levels which are not located near the ionization threshold $E = 0$ and possibly one level near this threshold. Another remark worth making is that the long distance behavior of our potential is $\sim \exp(-A_0 x)$ where $A_0 = \sum a_j + \sum b_j$ whereas the potential (6) tends to zero much faster, as $\sim \exp(-A_1 x^2)$.
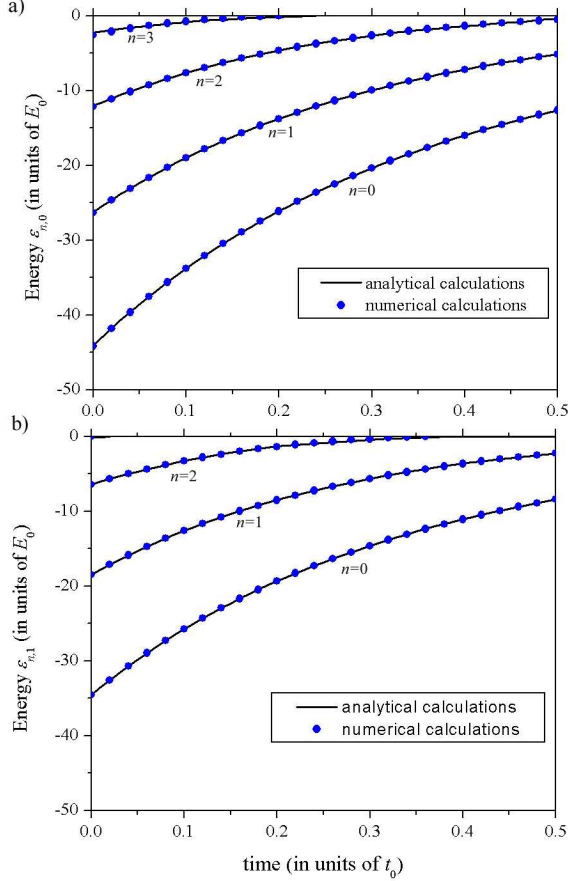
FIG. 2: (Color online) Energy spectra of electrons in NSPI QD with initial half-width $d = 1\mu m$ and $B_{hf}(r = 0, t = 0) = 2.65T$ as a function of time, $T_1/t_0 = 1$, $l = 0$ (a) and $l = 1$ (b). The solid lines are the energy levels obtained using the multisoliton approximate potential. The dots correspond to the energy levels, that were obtained as a numerical solution of the Shroödinger equation with the Gaussian potential.
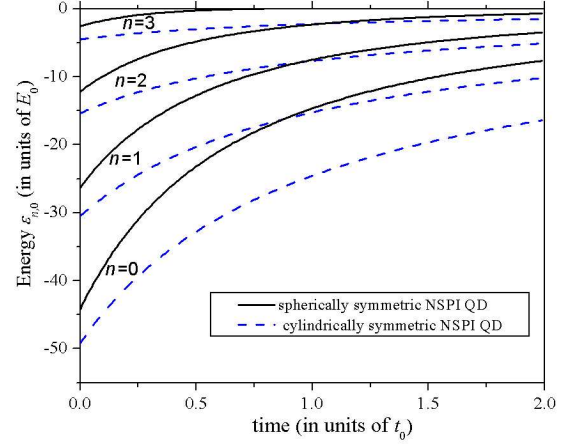
FIG. 3: (Color online) Energy spectra of electrons in NSPI QDs with spherical and cylindrical symmetry in the diffusive regime, $T_1/t_0 = 100$. The parameters of calculations are as on Fig. 2.

IV. RESULTS

The time dependence of the confining hyperfine field given by Eq. (3) determines the time-dependence of the electron energy levels in the NSPI QD. There are two characteristic times in the problem: the diffusion characteristic time t_0 and the relaxation characteristic time T_1. For $t \sim t_0 \ll T_1$ we distinguish diffusive regime, the times t such that $t \sim t_0 \sim T_1$ correspond to intermediate regime, and when $t \sim T_1 \ll t_0$ we are in relaxation regime. Here t is the observation time.

We found that the time-dependence of the energy levels in all regimes are qualitatively similar for NSPI QD with spherically symmetric confining potential: the number of energy levels, as well as their depth, decreases with time. It is interesting to note that the number of energy levels in cylindrically symmetrical NSPI QD in the diffusive regime remains constant [11], and the number of trans-

verse energy levels in NSPI QW in the diffusive regime even increases with time [11]. This remarkable fact is related to the symmetry of the confining potential: an increase of the symmetry results in a faster spreading of the confining potential due to the nuclear spin diffusion process.

In order to estimate the accuracy of our approximation, we compared the results obtained by supersymmetric transformations with numerical solutions of the Schrödinger equation with the Gaussian potential. We have used the Shooting Method to solve the radial Schrödinger equation, subjecting the solution to the following boundary conditions: $R_{n,l}(r \to 0) = r^l$ and $R_{n,l}(r \to \infty) \to 0$ which correspond to a discrete spectrum eigenfunction. It is convenient to define the function $P_{n,l}(r)$ as $R_{n,l}(r) = r^l P_{n,l}(r)$ thus reducing the first of the above conditions to $(\partial P_{n,l}/\partial r)|_{r=0} = 0$.

Figure 2 shows a representative result of our calculations. The time-dependence of the energy levels was calculated for NSPI QD based on GaAs with initial half-width $d = 1\mu m$ and $B_{hf}(r = 0, t = 0) = 2.65T$, corresponding to 50% nuclear spin polarization, in the intermediate regime, when $T_1/t_0 = 1$. The number of energy levels in the NSPI QD decreases with time. A comparison between analytical and numerical results shows that the method of supersymmetric transformations gives a good approximation for almost all energies except for a tiny interval near $E = 0$. This is clearly seen from Fig. 2(a) for $n = 3$ and Fig. 2(b) for $n = 2$ energy levels. Such a difference occurs because of different long distance asymptotics of the Gaussian and multisoliton potentials, discussed at the end of the Section III.

Faster spreading of nuclear spin polarization in the case of 3D diffusion than in the case of 2D diffusion results in qualitatively different behaviour of the energy spectrum

in NSPI QDs with spherical and cylindrical symmetry in the diffusive regime, as demonstrated in Figure 3 for $n = 0$. It is seen from Fig. 3 (this was exactly proved in Ref. [11]) that the number of energy levels in the cylindrically symmetrical NSPI QD in the diffusive regime is constant in time. In the case of spherically symmetric NSPI QD, the number of energy levels decreases in time.

V. CONCLUSIONS

We have investigated the electronic structure of a quantum dot created through a spherically symmetric local nuclear spin polarization within multisoliton potential approximation obtained by means of Darboux transformations. In particular, the electron energy spectrum of the NSPI QD having spherical symmetry was calculated as a function of time. We found a specific feature of the evolution of such NSPI QDs - the number of energy levels, as well as their depth, decreases with time in all regimes. This observation contrast with previously studied cylindrically symmetrical NSPI QD.

Moreover, it has been demonstrated that the approximation of a Gaussian potential by a multisoliton potential is much more efficient in comparison with the approximation by a parabolic potential. The parabolic approximation is acceptable only for the ground state, whereas multisoliton potentials give an excellent agreement with the exact results for all energies except for a tiny interval near $E = 0$. Moreover, for an electron confined by a multisoliton potential the wave function is given analytically. We would like also to point out that the method presented here can be applied for studying not only NSPI QDs but it also can be useful for describing, for instance, traditional quantum dots.

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